

STUDY ON THE EFFECT OF IGNITION LOCATION ON PRESSURE PILING.

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ABSTRACT

An explosion of flammable mixtures in interconnected compartments is commonly defined as pressure piling. Piling pressure is phenomenon when the peak pressure observed is higher than the predictable thermodynamic values. The two main mechanisms affecting pressure piling are pre-compression and violence of explosion. Therefore, this paper is aim study on the effect of ignition location on pressure piling using Computational Fluid Dynamic (CFD) simulation. Different points of ignition were studied using this simulation which are central and end point in the interconnected vessel (primary vessel). Besides that the role played by pre-compression and violence of explosion were also studied. In this studied, CFD codes were used as this simulation able to reproduce the explosion phenomenon (propane air) strongly depends on the sub-models used for turbulence and combustion. The proportion of the propane air used was 50-50

.The model of the interconnected vessel were construct in the Gambit with the height and width of the primary vessel are 0.75cm and 0.305. Meanwhile the height and width of the secondary vessel are 0.15cm and 0.26cm. Later on, the model was imported to the Fluent to reproduce the explosion. From my research, the peak pressure for ignition location at the end in the primary vessel gives the highest value than the peak pressure of central ignition location. This is due to the end ignition location; the flame has much more time to develop turbulence before it enters the secondary vessel. This method is the best to study about an explosion in interconnected vessel because of low cost involve rather than sacrifice a plant which is something irrational to be done. From this study we can clearly see that the end ignition location produced higher peak pressure than the central ignition location due to the development of the turbulence intensity.

Key words: *pressure piling, interconnected vessel, explosion, propane air, Computational Fluid Dynamic (CFD), pre-compression and violence of explosion*

TABLE OF CONTENTS

SUPERVISOR’S DECLARATION	IV
STUDENT’S DECLARATION	V
<i>Dedication</i>	VI
ACKNOWLEDGEMENT	VII
ABSTRACT	VIII
ABSTRAK	IX
TABLE OF CONTENTS	X
LIST OF FIGURES	XI
LIST OF TABLES	XII
LIST OF ABBREVIATIONS	XIII
LIST OF ABBREVIATIONS	XIV
1 INTRODUCTION	1
1.1 Motivation and statement of problem	1
1.2 Objectives	2
1.3 Scope of this research	2
1.4 Main contribution of this work	3
1.5 Organization of this thesis	3
2 LITERATURE REVIEW	5
2.1 Concept of pressure piling	5
2.2 Previous studies on pressure piling	5
2.3 Location Of Ignition Source and Volume ratio	5
2.4 Violence of explosion and pre-compression	5
2.5 Laminar flames	6
2.6 Turbulence	
3 METHODOLOGY	7
3.1 Overview	7
3.2 RANS-Based Model	7
3.3 Simulation Model and Parameters	7
4 RESULTS AND DISCUSIONS	9
4.1 Comparison on peak pressure for center and end ignition	9
4.2 Comparison on mass fraction for center and end ignition	9
4.3 Comparison on turbulent kinetic for center and end ignition	9

6	CONCLUSION.....	11
6.1	Conclusion.....	11
	REFERENCES	12

LIST OF FIGURES

Figure 2.1.1: Typical pressure curves from a pressure piling situation. Pressure in the secondary chamber (red) rises steadily until the flame arrives and a very fast combustion occur. At the point where the curves intersect flow direction trough the opening is reversed (Rogstadkjernet, 2004).	15
Figure 3.3.1: The simulation model mixtures of air-propane in interconnected vessels.	21
Figure 4.1.1: The simulation model mixtures of air-propane in interconnected vessels.....	21
Figure 4.1.2: Graph on pressure for central ignition location.....	22
Figure 4.1.3: Graph on pressure for end ignition location.....	23
Figure 4.2.1: The simulation model mixtures of air-propane in interconnected vessels.....	23
Figure 4.2.2 : Graph on mass fraction for central ignition point	24
Figure 4.2.3 : Graph on mass fraction for end ignition point	25
Figure 4.3.1: The simulation model mixtures of air-propane in interconnected vessels.....	25
Figure 4.3.2 : Graph on turbulent kinetic energy for central ignition location.....	26
Figure 4.3.3 : Graph on turbulent kinetic energy for end ignition location	26

LIST OF TABLES

Table 2.1.1: Previous study on pressure piling	8
Table 3.3.1 below shows the parameter used in the simulation.....	9
Table 3.3.2 the location of the ignition	9

NOMENCLATURE

C_t	dimensionless constant
D	turbulent diffusion coefficient, $\text{m}^2 \text{s}^{-1}$
d_p	pipe diameter, m
$[dP/dt]$	rate of pressure rise, bar s^{-1}
f	ratio of pipe cross section to vessel volume, $\text{m}^2 \text{m}^{-3}$
L_t	turbulence macroscale, m
P	pressure, bar
R_c	combustion rate, $\text{kg m}^{-3} \text{s}^{-1}$
S_t	turbulent burning velocity, m s^{-1}
S_l	laminar burning velocity, m s^{-1}
u'	turbulence intensity, m s^{-1}
v_x	axial gas velocity, m s^{-1}
x_{lim}	minimum mass fraction in
χ	turbulisation factor
ν	kinematic viscosity, $\text{m}^2 \text{s}^{-1}$
ρ	mixture density, kg m^{-3}

LIST OF ABBREVIATIONS

CFD	Computational fluid dynamics
DES	Detached eddy simulation
RANS	Reynolds averaged Navier-Stokes
SA	Spalart-Allmaras model
SST	Shear stress transport model

INTRODUCTION

Background of study

Explosion of flammable hydrocarbon-air mixtures in two or more interconnected vessels is commonly occurred in industry nowadays. This phenomenon is called as 'pressure piling'. According to Beyling (1906), the term pressure piling is referring to situations in which the pressure in one chamber has increase prior to its ignitions. Pressure piling is a situation where the peak pressure is higher than the predictable by thermodynamic are observed. This explosion is recognized as a major source of risk in industry as this explosion consists of flammable gaseous. Bartknecht (1981); Phylaktou and Andrews (1993), stated that the explosions show an anomalous destructive power deriving from rates of pressure rise and peak pressures much higher than those corresponding to explosions in single closed vessels. Several parameters that could affect the intensity of pressure piling have been found from the previous work. Abdullin, Babkin, & Senachin, (1988); Bartknecht, (1981);Beyling,(1906);Gleim & Marcy, (1952) and Maremonti,Russo,Salzano and Tufano,(1999) proposed in their findings that tube area and ratio of volumes of the interconnected vessels strongly influence the intensity of the pressure piling. Besides that, according to Grice & Wheeler, (1929); Phylaktou & Andrews, (1993) and Singh ,(1977) also showed that the intensity of pressure piling is affected by location of the ignition point. The main mechanisms affecting the pressure piling are pre-compression and violence of explosion (Di Benedetto & Salzano, (2010).

Motivation and statement of problem

Simple situations of an explosion can be a complex task as it is intrinsically unsteady and strongly influenced by the feedback arising between flame, flow-field and geometry. Benedetto and Salzano (2010) stated that pressure generated by the combustion wave (explosion) will be depend on how fast the flame propagates and how the pressure can expand away from the gas cloud. In result, semi-empirical mathematical models (lumped parameter) by Abdullin et al.,(1998) and Singh,(1994) was proposed. This model describes the main features of the explosion and allows the pressure-time behavior to be computed. Besides that, two “turbulisation factors” (x_1, x_2) are introduced to describe the flame front wrinkling ,respectively in the ignition and in the secondary vessel. However, their applicability is mainly restricted to the experimental conditions in which they are validated. Therefore, an alternative approaches are based on the solution of the Navier-Stokes equations, coupled to the conservation equations for mass and energy. Hence, CFD simulation is used to solve the Reynolds Averaged Navier-Stokes (RANS) equations. The ability of RANS-based CFD model to reproduce the explosions phenomenon is strongly depends on the sub-models used for turbulence and combustion. Basically, the CFD codes are based on simplified laminar combustion model and on the derivation of the well-known EBU model (Spalding, 1977) for describing turbulent combustions. These codes are mainly on interaction between obstacles and flame propagation in estimating the pressure peak reached in equipment. However, according to Popat. et al., (1997) few empirical coefficients has to be tuned in order to give reasonable result. Maremonti et al. (1999) used the commercial CFD code AutoReaGas (van den Berg, The, Mercx, Moilleau and Hayhurs, 1995) to reproduced pressure piling phenomenon using a commercial code specifically developed for simulating gas explosions ,based on the so-called quasi-laminar approach (Bakke, 1986) and the Eddy Dissipation combustion model (Magnussen and Hjertager, 1977). The code was able to simulate the observed phenomenon provide that some parameters in the combustion model are adjusted to reproduce the complex phenomenon of pressure piling. Here, a RANS-based CFD model and a combustion model without any modified parameter will be used.

Objective

The following is the objective of the research:

- To study the effect on ignition location (center and end) on pressure piling.

Scope of this research

The following are the scope of this research:

- A RANS-based CFD model and a combustion model are used
- Two different ignition locations which are end and center ignition position in interconnected vessel will be used to study the effect on pressure piling
- The role played by pre-compression and violence of explosion on pressure piling will be studied.

Main contribution of this work

The following are the contributions

- An explosion in interconnected vessels during reaction process could be avoided because the parameter, the effect of ignition source, which lead to an explosion to occur is studied. The explosion will totally effect the environment and also people. Therefore, using this software, the explosion can be avoided.
- Interconnected vessels can be made which could withstand the parameter that lead to gas explosion. Thus, will increase the safety level in the plant area.

Organization of this thesis

The structure of the reminder of the thesis is outlined as follow: Chapter 1 provides a description about the objective and scope of the project and also explains on the contribution of this project to the people and the environment.

Chapter 2 gives a review about the concept of pressure piling. Besides that, in chapter 2 also include the previous studies done by researchers on pressure piling. The parameter which lead to pressure piling, location of ignition source, being discussed in detail in this chapter. In addition, the two important mechanisms, pre-compression and violence of explosion are also discussed.

Chapter 3 is about the method and material that is being used in this project. The detail of how to run the software is discussed in this chapter. The condition to run the software is also being discussed. The parameter that will be used is also stated in this chapter. The simulation model of this project is also shown in this chapter,

Chapter 4 is the preliminary task where the expected result is shown in 2D simulation.

Lastly in chapter 5 shows the result from the Computational Fluid Dynamic simulation on the explosion in the interconnected vessel with different ignition location: center and end.

2 LITERATURE REVIEW

2.1 Concept of pressure piling

Explosion may be defined by combustion of ‘premixed’ combustible mixture (gas cloud), causing rapid increase in pressure. The pressure generated by the combustion wave is depending on how fast the flame propagation and how the pressure could expand away from the gas cloud. There are several type of explosion such as vapour liquid explosion, boiling liquid expanding vapour explosion (BLEVE), detonation and pressure piling.

Simple situations of an explosion can be a complex task as it is intrinsically unsteady and strongly influenced by the feedback arising between flame, flow-field and geometry. Benedetton and Salzano (2010), stated that pressure generated by the combustion wave (explosion) will be depend on how fast the flame propagates and how the pressure can expand away from the gas cloud. In result, semi-empirical mathematical models (lumped parameter) by Abdullin et al (1998), and Singh (1994), was proposed. This model describes the main features of the explosion and allows the pressure-time behavior to be computed. Besides that, two “turbulisation factors” (x_1, x_2) are introduced to describe the flame front wrinkling ,respectively in the ignition and in the secondary vessel. However, their applicability is mainly restricted to the experimental conditions in which they are validated. Therefore, an alternative approaches are based on the solution of the Navier-Stokes equations, coupled to the conservation equations for mass and energy. Hence, CFD simulation is used to solve the Reynolds Averaged Navier-Stokes (RANS) equations. The ability of RANS-based CFD model to reproduce the explosions phenomenon is strongly depends on the sub-models used for turbulence and combustion. Basically, the CFD codes are based on simplified laminar combustion model and on the derivation of the well-known EBU model (Spalding, 1977) for describing turbulent combustions. These codes are mainly on interaction between obstacles and flame propagation in estimating the pressure peak reached in equipment. Unfortunately, according to Popat et al. (1997), few empirical coefficients has to be tuned in order to give reasonable result. Maremonti et al. (1999), used the commercial CFD code AutoReaGas (Berg et al., 1995) to reproduced pressure piling phenomenon using a commercial code specifically developed for simulating gas explosions ,based on the so-called quasi-laminar approach (Bakke,1986) and the Eddy Dissipation combustion model (Magnussen and Hjertager,

1977). The code was able to simulate the observed phenomenon provide that some parameters in the combustion model are adjusted to reproduce the complex phenomenon of pressure piling. This paper presents the simulation studies on the effect of different ignition location in interconnected vessel on pressure piling. Pressure piling is referred to a situation in which one chamber has increased the pressure prior to its ignition. During combustion initiated inside a closed vessel, a finite amount of energy is released and the system will at any time be defined by the equation of state:

$$pV=nRT$$

Equation (1)

According to Di Benedetto and Salzano (2010), in closed vessel, combustions wave propagation is attended by a rise in pressure and mass flow which is directed from the later toward the point of ignition. Due to turbulence induced by gas expansion and interaction with geometry, transition from the laminar flame to the turbulent flame may be occurring. The temperature and pressure of the unburned gas will rise according with the law of adiabatic compression as a result there will be a temperature gradient between the gas burned first and the gas burned last. Initially, the gas expands at a constant pressure and is subsequently compressed almost to its original volume as the part of gas is consumed. In primary vessel, the flame propagates is a laminar. When the flame reaches the secondary vessel it will encounter a compressed turbulent mixture. Time between ignition and flame arrival in the secondary vessel and volume of the two chambers will decide what pre-ignition pressure will be at this time. Increase in turbulence level will distribute to radical species and heat, resulting in a rapid combustion process.

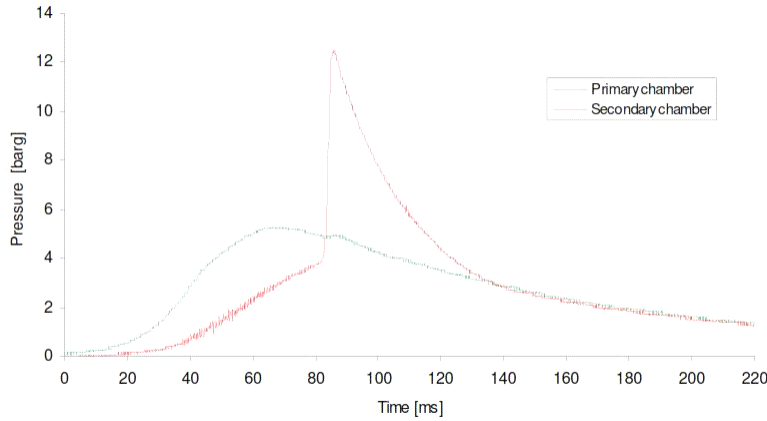


Figure 2.1.1: Typical pressure curves from a pressure piling situation. Pressure in the secondary chamber (red) rises steadily until the flame arrives and a very fast combustion occur. At the point where the curves intersect flow direction through the opening is reversed (Rogstadkjernet, 2004).

2.2 Previous studies on pressure piling.

Numerous researches had been done on pressure piling. Table 1 shows the previous studies of pressure piling.

Table 2.1.1: Previous study on pressure piling

Author	Year	Objective
A.Di Benedetto, E.Salzano & G.Russo	2005	Predicting pressure piling by semi-empirical correlations
Razus, D.,Oncea,D.,Chirila,F.,& Ionescu,N. I	2003	Transmission of an explosion between linked vessel
Abdullin, R.K,Babkin ,V.S.,&Senanchin,P.K	1998	Combustion of gas in connected vessels
P.A. Libby, & F. A. Williams	1996	Turbulence reacting flow
Popat,N.R.,Catlin,C.A.,Arntzen,B.J et al	1996	Investigations to improve and asses the accuracy of computational fluid

		dynamic based explosion models
Singh,J	1994	Gas explosion in interconnected vessels
Libby ,P.A., & Williams,F.A	1994	Turbulence reacting flows
Marenmonti,M.Russo & Tufano,V	1994	Numerical simulation of gas explosions in linked vessel
Gulder,O.L	1990	Turbulent premixed propagation models for different combustion regimes
W.C.F Shepherd	1988	Ignition of gas mixtures by impulsive pressure
Borghi,R.	1988	Turbulent combustion modeling
Bakke,J.R	1986	Numerical simulation of gas explosion in two-dimensional geometries
N. Kawaguchi, O.Takeshi Sato, G.	1985	Premixed flame propagation models for different combustion regimes

2.3 Location of ignition source and Volume ratio

Previous work by Domina Razus et al., (1998) found that the explosion transmission between linked vessels is strongly depends on vessels volume ratio and position of the ignition source.

An experiment has been done by Singh (1984) proved the importance of ignition location source and volume ratio in pressure piling. From the experiment, the peak pressure in the secondary vessel can be severely affected by the position of the ignition in the first vessel. However, his result is it not suitable to be used since Singh did not change the size of the transfer opening.

Maremonti,et al. (1999) investigated the ability of a CFD code (AutoReaGas) to model gas explosions in linked vessels. Basis for their simulation was the experiments conducted by

Phylaktao et al (1993), but as previously noted the volume ratio in these was 1:1 and no actual pressure piling occurred. However, the code was able to take into account the effect of different ignition location (central and end ignition). The agreement between measured and calculated data was good regard to the peak pressure but less accurate for the rate of pressure rate and flame speed. The computed values of the turbulence intensity in both chambers demonstrated that turbulence induced in the secondary vessel is a major factor affecting explosion violence. This parameter was strongly affected by the distance between the ignition source and inlet pipe in the interconnected vessel.

Besides that Di Benedetto and Salzano (2010), also stated that the higher is the distance between ignition point and the duct entrance, the higher the peak pressure.

2.4 Violence of explosion and pre-compression

The mechanisms affecting the pressure piling are the violence of explosion and pre-compression. Benedetto and Salzano (2010) found during propagation in the first vessel, pressure increases and a flux of unburned gases from the first vessel towards the second occur. The mass flux from the first vessel towards the second causes and increases of pressure in the second vessel. Consequently, when the flame enters the second vessel, ignition occurs at an initial pressure which is higher than the atmospheric pressure. The increase of initial pressure has a dramatic effect on the pressure peak as it is strongly coupled to the violence of explosion in the second vessel.

According to Maremonti et al. (1999) the induced turbulence in the secondary vessel is a major factor affecting the explosion violence. Molkov, Dobashi, Suzuki, and Hirano (2000) proposed a turbulent Bradley number (Br_t), the ratio of reaction time to venting time for turbulent flame propagation. Di Benedetto and Salzano (2010) stated that at low values of turbulence level i.e. very high Br_t numbers (Br_t approaches infinity), reaction time is much lower than the venting time and the peak pressure can be significantly lower than the thermodynamic value corresponding to the pressure in the secondary vessel at ignition time. Increasing the volume ratio results in a more intense pre-compression (pressure in the secondary vessel at ignition time

increases) thus suggesting that ignition in the second vessel occurs starting from a higher value of pressure. Consequently, at a fixed level of turbulence, the peak pressure should be higher.

2.5 Laminar Flames

Reaction rate, thermal and molecular diffusivity are fundamentally tied to the subject of flame propagation as shown in equation (3.2). A scheme of the reaction zone showing characteristic gradients of temperature and concentrations is given in Figure 2.5.1 :

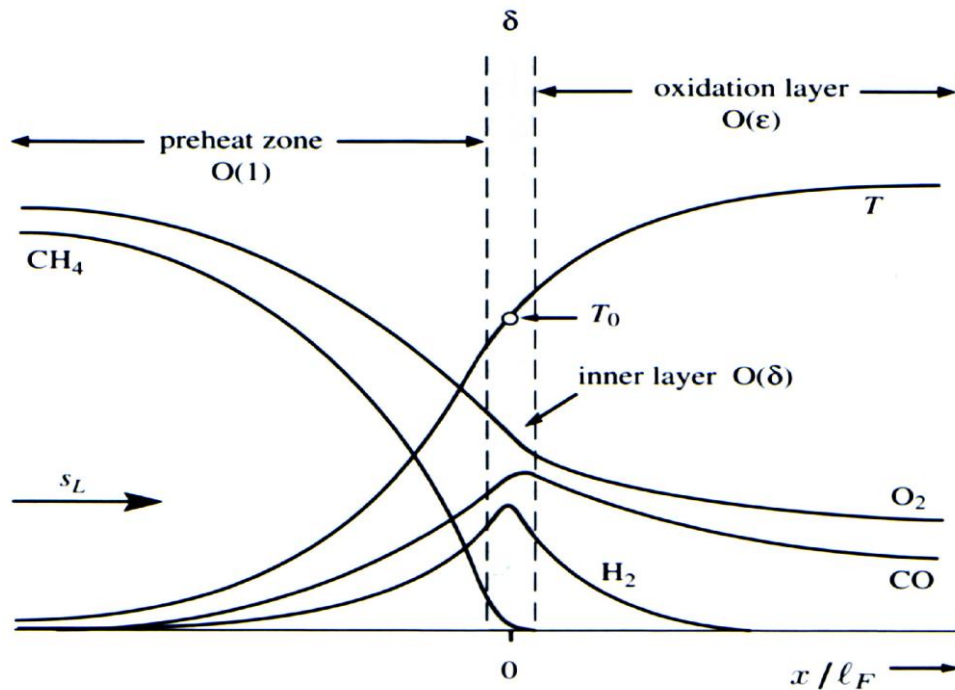


Figure 2.5.1 Schematic illustration of the reaction zone for a methane-air mixture. The fuel consumption zone denoted δ is where the fuel is consumed and the radicals are depleted by chain breaking reactions. (Illustration from Peters 2000)

There are three main branches of theories used for the description of flame propagation: thermal theory, the comprehensive theory and the diffusion theory. As the name indicates different emphasis is placed on the diffusive characteristics. The comprehensive theory, which is derived from the species conservation and energy equations, rank as the better of three and is more able

to explain trends in flame propagation speeds. The expression for laminar burning velocity, SL , for a first order reaction is given as:

$$S_L \sqrt{\frac{2\lambda_f C_{pf} A}{\rho_0 C_p^2} \left(\frac{T_0}{T_f}\right) \left(\frac{n_r}{n_p}\right) (Le) \left(\frac{R_u T_f^2}{E_a}\right)^2 \left(\frac{e^{-E_a/R_u T_f}}{(T_f - T_0)^2}\right)} \quad (1)$$

However, the inherent difficulties in assessing diffusive properties and reaction rates reduce the usefulness of these models, and one is left to depend on experimental values for burning velocities. Figure 2.3.2 shows some experimental data for the burning velocity of hydrogen mixtures and indicates the uncertainty involved.

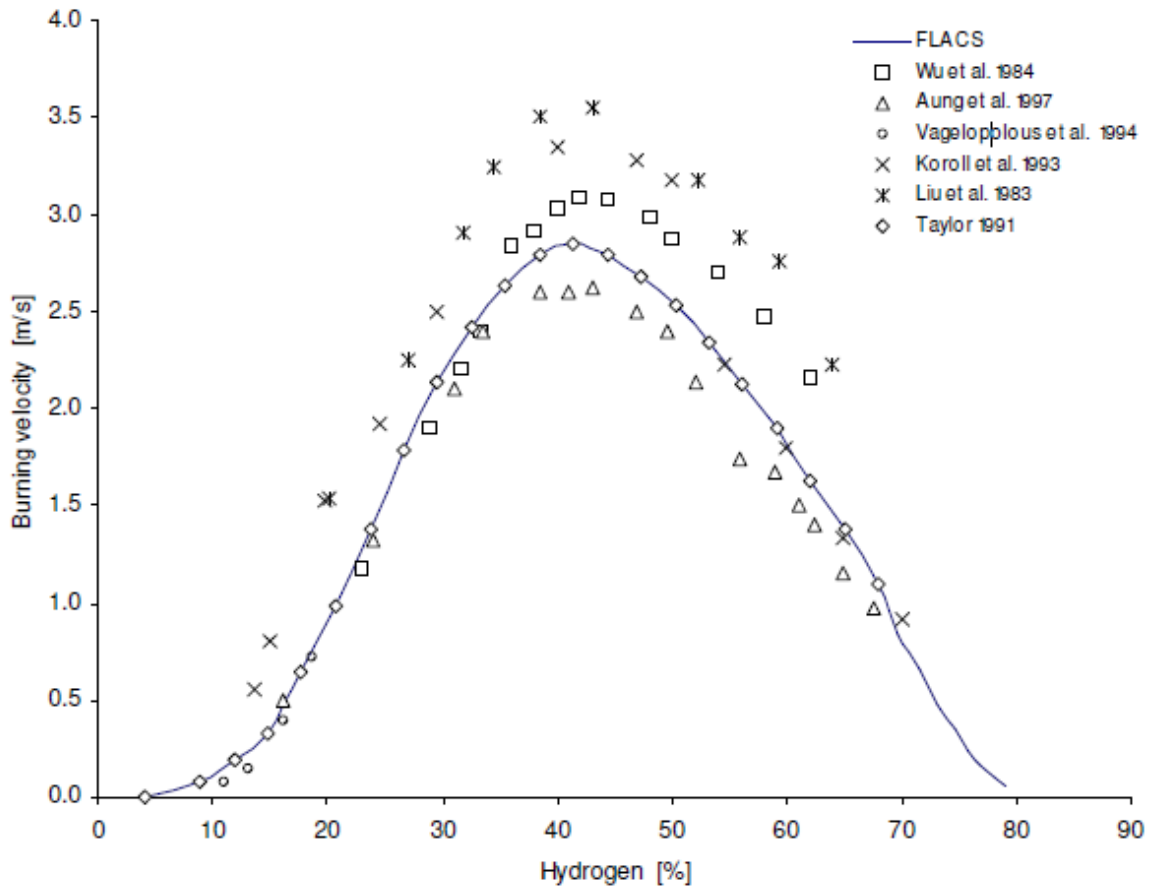


Figure 2.5.2 Experimentally determined burning velocities for hydrogen/air mixtures.

Several methods can be used to determine burning velocity from experimental pressure data and for combustion in a closed spherical vessel the following equation can be used (Skjold 2003, Dahoe 1996):

$$S_{L,ip} = \frac{1}{3p_m} \left(\frac{dp}{dt} \right)_m V_v^{1/3} \left(\frac{3}{4\pi} \right)^{1/3} \left(1 + \frac{p_{ip}}{1[bar]} \right)^{-1/\kappa} \left\{ 1 - \left(1 - \frac{p_{ip}}{p_m} \right) \cdot \left(1 + \frac{p_{ip}}{1[bar]} \right)^{-1/\kappa} \right\}^{-2/3} \quad (3.10)$$

Where:

Subscript ip denotes the inflection point on the pressure curve (d²p/dt²)

pm denotes measured pressure

Vv denotes vessel volume

k denotes specific heat ratio (cp/cv)

Equation 3.10 is based on a few idealized assumptions (ideal gas behaviour, thin flame, fast reaction, no flame wrinkling) and only applies for central ignition. As already indicated the burning velocity will be significantly affected by changes in temperature and to a lesser extent by changes in pressure. The increase in kinetic energy as a result of higher temperature reduces the energy needed to initiate reaction in the unburned gas and thereby enhance burning velocity. Although generally surpassed by the effect of increased temperature, elevation of pressure has the opposite effect. Laminar burning velocity, S_L , as function of T and P can be expressed by:

$$S_L = S_{L0} \left(\frac{T_R}{T_0} \right)^\alpha \left(\frac{P}{P_0} \right)^\beta \quad (2)$$

Where subscript 0 denotes reference state and TR is temperature in reactants. Values for α and β are significantly affected by equivalence ratio (Metghalchi and Keck 1980) and, to a lesser degree, pressure (Shebeko, Tsarichenko et al. 1991). Table 2.3.3 shows some selected values for α and β .

	Methane [1]	Propane [1]	Acetylene [2]	Hydrogen [2]
α	2.0	2.13	2.0	1.26
β	-0.5	-0.17	-0.06	0.26

Table 2.5.3 Empirical values for the exponents in equation (3.11) [1] (Metghalchi and Keck 1980) [2] (Milton and Keck 1984) Note how temperature and pressure dependency deviates for hydrogen and hydrocarbons.

It should be noted that the equation and constants given apply for stoichiometric mixtures. Experiments performed by Strauss and Edse (1958), imply that values for β should be reduced for rich mixtures and increased for lean mixtures. This observation is also in agreement with the theory of diffusional stratification that is prone to occur in stoichiometrically unbalanced mixtures in which the diffusivity of the deficient component exceeds that of the excess component (Lewis 1987). This causes instability in the flame front and may result in a cellular boost of measured burning velocity.

In general, burning velocity S_L is considered to be a direct function of properties of the combustible mixture and depends neither on geometry nor flow. This is not absolutely true for the diverging flame propagation immediately after ignition. The curvature of the flame sphere results in higher diffusive losses, which in turn lowers the temperature in the reaction zone and burning velocity. The effect will rapidly diminish as the flame sphere grows and is often neglected. Although the effect is small the critical flame diameter (or quenching diameter) indicates that methane mixtures would be relatively more affected than hydrogen. Although flame stretch is of limited importance for laminar flames it gains significant relevance as flames become turbulent.

2.6 Turbulence

Turbulence is not a feature of fluids but of fluid flows and most of the dynamics of turbulence does not depend on fluid characteristics. Although fluid properties as mass and viscosity do affect turbulence such a discussion would be outside the scope of this text. Turbulent processes occur at different length scales and are useful parameters for characterizing turbulent structure. The largest length scale, l_L , corresponds to the geometrical dimensions of the system. The integral length scale, l_0 , is the characteristic length scale of eddies containing most of the kinetic energy and is closely tied to l_L . The Kolmogorov length scale l_η denotes dimensions of the smallest turbulent structures. At the Kolmogorov length the time needed for an eddy to rotate half a revolution is equal to the diffusion time across the diameter l_η , therefore turbulent transport does not extend below l_η . The Kolmogorov length scale is defined as a function of kinematic viscosity, ν , and dissipation rate, ϵ .

$$l_\eta = \left(\frac{\nu^3}{\epsilon} \right)^{1/4} \quad (4)$$

The Taylor micro scale l_λ is the ratio of time scale of large and small eddies and is associated with the dissipation of turbulent energy. k denotes kinetic energy.

$$l_\lambda^2 = 10\nu \frac{k}{\epsilon} \quad (5)$$

The distribution of the kinetic energy among the spectrums of eddies with different diameters is described by the turbulent energy spectrum and shown in Figure 3.3. The energy spectrum has its peak at the integral length scale, l_0 , and ends at the Kolmogorov length l_η scale.

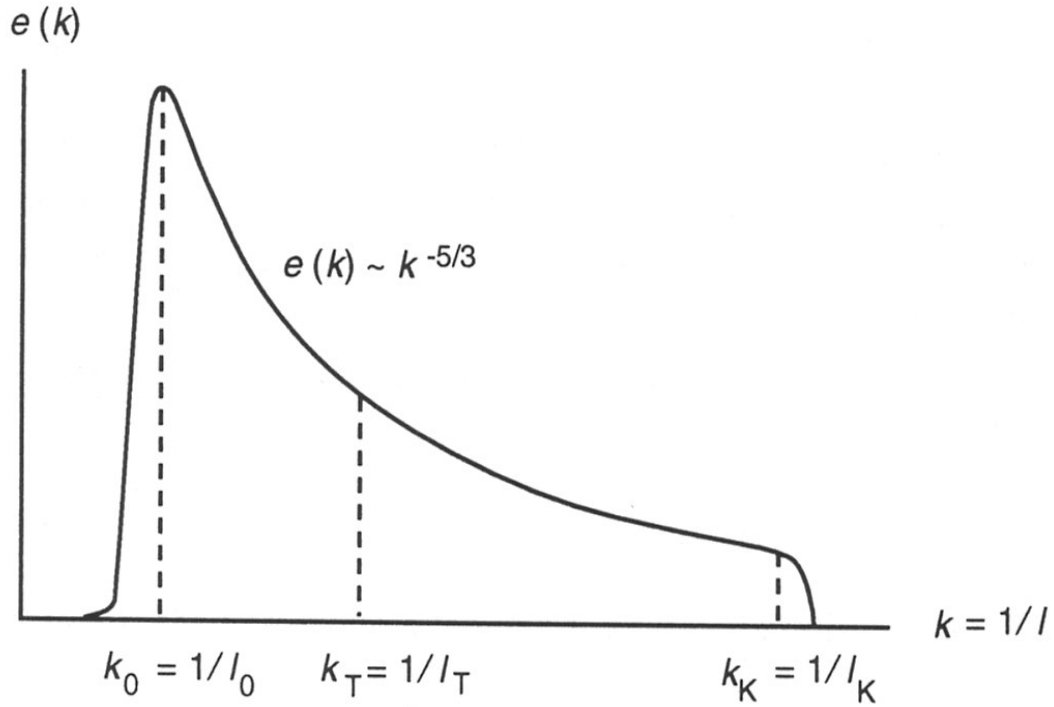


Figure 2.6.1 *Turbulent energy spectrum showing the energy cascade.*

Turbulent flow results when instabilities in a flow are not sufficiently damped by viscous action and the fluid at each point in the flow exhibits random fluctuations. Reynolds number can be considered as a ratio between a destabilizing momentum and a stabilizing or damping, viscous effect.

$$Re = \frac{\rho u l}{\mu} \quad (6)$$

where u denotes velocity and l is the characteristic length of the system (diameter in tube flow). Together with the Kolmogorov length scale it can be used to define the turbulent Reynolds number, Re_t . Since Re_t is based on properties of the turbulence it is associated more closely with regimes and dynamics of turbulent motion than Re . Re_t is given as:

$$\text{Re}_t = \frac{\bar{\rho} \sqrt{2k} l_0}{\bar{\mu}} = \left(\frac{l_0}{l_\eta} \right)^{4/3} \quad (7)$$

Where k denotes the kinetic energy.

When turbulent are initiated in a fluid it will first be present as large anisotropy eddies. Due to vortex stretching, eddies break up and fission into smaller and smaller eddies which simultaneously becomes faster and more isotropic. As eddies get smaller the strain rates increase. The intensity of fluid fields is characterised by the root mean square, u' , of the velocity fluctuations. It is often expressed as a percentage of the mean velocity and may amount to 10% in very turbulent fields (McCabe, Smith et al. 1993). In practical situations the intensity usually varies with each component of velocity and have significant spatial variations. In strict sense u' is only relevant for isotropic turbulence. The kinetic energy of turbulence, per unit mass, is defined as:

$$k = \frac{1}{2} \left[\overline{u^2} + \overline{v^2} + \overline{w^2} \right] \quad (8)$$

Characterizing turbulence by such simple measures as described above have obvious limitations. Turbulence is a highly three dimensional and time dependent phenomena and especially high spatial and transient variations must be anticipated in pressure piling situations.

3 METHODOLOGY

3.1 Overview

This paper is about studying the effect of ignition point during pressure piling using Computational Fluid Dynamics (CFD). A combustion model with a 50-50 in proportion of propane and air was used in aiming for turbulence induced by gas expansion and interaction with geometry, transition from the laminar flame to the turbulent flame may occur. This software normally used to solve equation for mass, momentum, energy and species mass fraction. This CFD tool is used to determine the effect of different ignition location in primary vessel in interconnected vessel during pressure piling. First and foremost, a 2D-simulation was performed for central ignition location in the primary vessel. The first 2D –simulation for central ignition location is done where the ignition point is at 0.35 at the x-axis and 0.15 at the y-axis. Then, the meshed is import to the Gambit to get the results on mass fraction, turbulent kinetic and peak pressure. The second 2D simulation is done for end ignition location where 0.13 for x-axis and 0.12 for y-axis. Then, the meshed is import to the Gambit to get the results. The result of both ignition locations is being compared and a conclusion is derived It is clear from the modeling exercise performed in this work that CFD is a promising method for modeling a pressure piling in the interconnected vessel. Furthermore, the CFD method is certainly less expensive than the experimental characterization studies.

3.2 RANS-based model

In the paper here presented, CFD codes are used in solving Reynold Averaged Navier-Stokes (RANS) equations. CFD codes are used because this simulation able to reproduce the explosion phenomenon (propane and air) strongly depends on the sub-models used for turbulence and combustion. The model used is based on the unsteady Reynolds average energy, momentum and mass balance equation.

Continuity Equation:

$$\frac{\partial \bar{\rho}}{\partial t} + \frac{\partial}{\partial x_j} (\bar{\rho} \tilde{u}_j) = 0$$

Equation (2)

Momentum balance equation:

$$\frac{\partial (\bar{\rho} \tilde{u}_i)}{\partial t} + \frac{\partial}{\partial x_j} (\bar{\rho} \tilde{u}_j \tilde{u}_i) = -\frac{\partial \bar{P}}{\partial x_i} - \frac{\partial}{\partial x_j} (\overline{\rho u_j'' u_i''})$$

Equation (3)

Energy balance equation :

$$\frac{\partial (\bar{\rho} \tilde{e})}{\partial t} + \frac{\partial}{\partial x_j} (\bar{\rho} \tilde{u}_j \tilde{e}) = -\bar{P} \frac{\partial \tilde{u}_j}{\partial x_j} - \frac{\partial}{\partial x_j} (\overline{\rho u_j'' e''})$$

Equation (4)

Progress variable equation:

$$\frac{\partial (\bar{\rho} \tilde{c})}{\partial t} + \frac{\partial}{\partial x_j} (\bar{\rho} \tilde{u}_j \tilde{c}) = -\bar{\omega} - \frac{\partial}{\partial x_j} (\overline{\rho u_j'' c''})$$

Equation (5)

Where ρ, P, u, c and e are respectively the density, the pressure, the velocity, the progress variable and the internal energy. The overbars ($\bar{}$) and ($\tilde{}$) denote Reynolds and Favre average quantities respectively and (\prime) represents fluctuating variables.

A commercial CFD solver (CFD-ACE+) was used for the numerical solution. The transient calculations were performed by means of the Crank-Nicholson scheme. The Courant condition control for time-stepping was used for the evaluation for the maximum time step (Morton & Mayers, 1994) :

$$\Delta t = CFL \frac{\Delta l}{|u| + c}$$

Equation (6)

From this study, peak pressure in the secondary vessels will be observed. The peak pressure is affected by the position in the first vessel. According to Bartknecht et al (1981), the higher the distance the distance between ignition source and the duct entrance, the higher the pressure.

3.3 SIMULATION MODEL AND PARAMETERS

Figure 1 shows the simulation model of primary vessel diameter and length is 0.705 cm and 0.305 cm. Meanwhile for the secondary vessel, the diameter and width are 0.15cm and 0.26cm. This interconnected vessel is in simulation scale. Both vessels were connected with a tube or pipe which the length and diameter of the pipe are 0.26cm and 0.051cm. The first ignition (end) was located at point of 0.12 at y-axis and 0.13 at the x-axis. The computational grid has a total of 54200 cells with minimum spacing of 0.01 cm. This method is then repeated with different ignition location which is 0.35 at x-axis and 0.15 at y-axis.